JÜLICH
FORSCHUNGSZENTRUM

Hierarchical parallelisation of functional renormalisation group calculations

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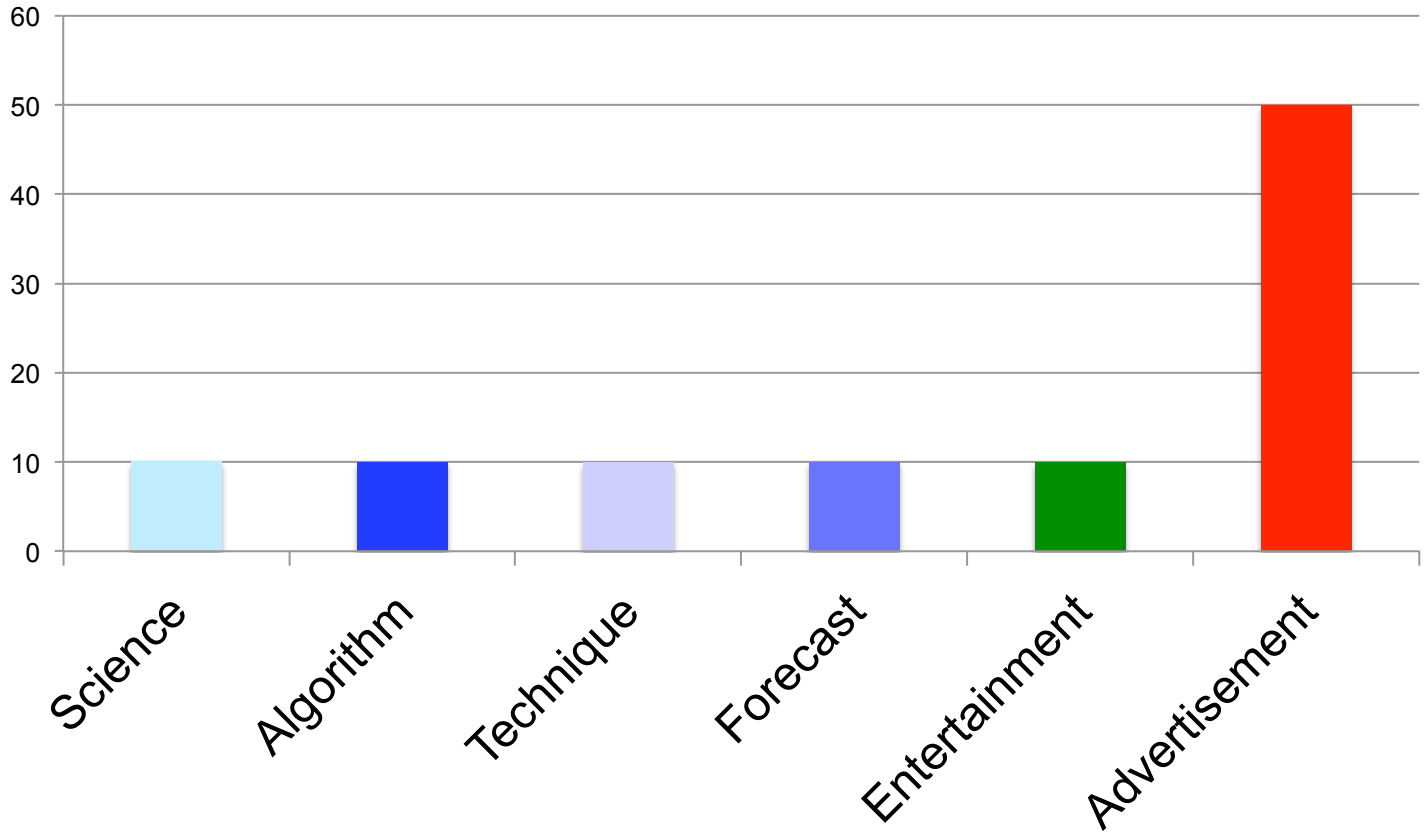
Distribution Function of this Talk



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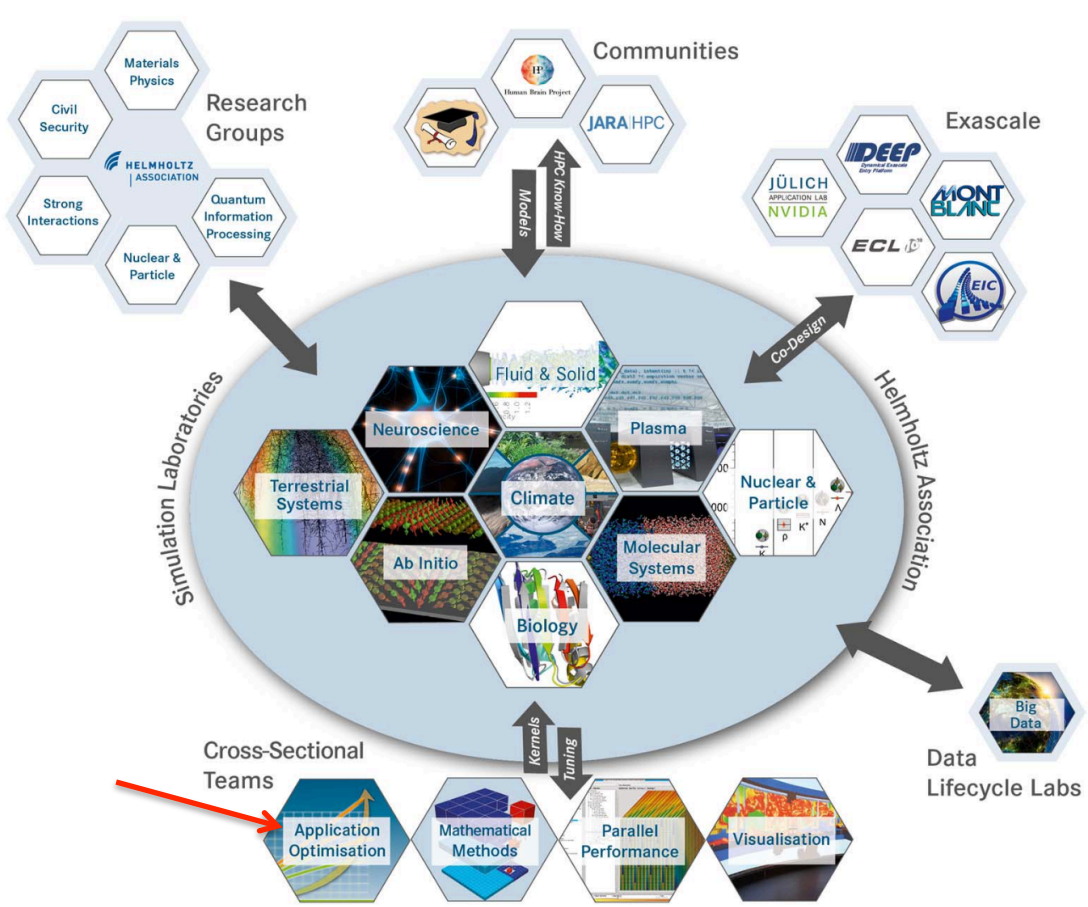
Where we are within JSC ...



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... what we do ...

On the web site:

“The cross-sectional team "Application Optimization" is responsible for the optimization and petascaling of applications in terms of performance, efficiency and parallel I/O. We provide users with knowledge and proper tools sets for their work on the Jülich HPC systems. We strongly interact with the Simulation Laboratories as well as the Cross-sectional teams "Methods and Algorithms" and "Performance Analysis". [...]”

In short: We help scientists to make proper use of (not only) our HPC systems

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... and why we offer this talk

We here report on an in-house example of such a scaling and optimisation process, hoping to generate interest in the audience.

Our goal: To get in contact with scientists within the IAS who could benefit from our services.

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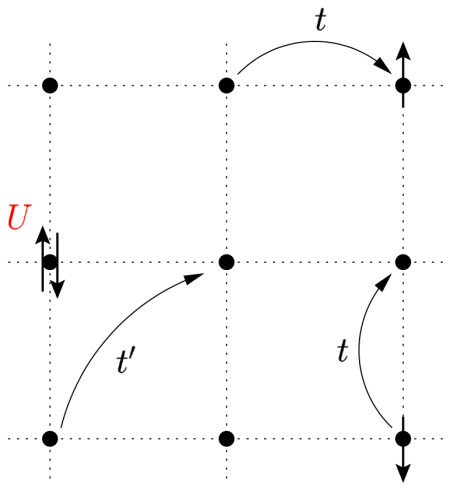
Physical Context: Model and Method



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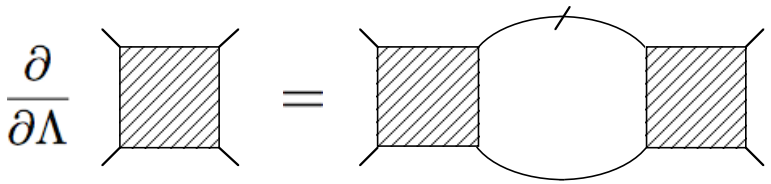

2d Hubbard Model for
Electrons on a Square Lattice

Functional Renormalisation Group:
1-loop equation for effective Interaction

captures e.g. competitive interplay of magnetism and superconductivity
in the weak-coupling regime

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Technical Task: Solve large ODE

let V[i] be a 1d array in which ALL coupling constants are stored.

Then a natural computational unit is given by calculating the rhs for one single element:

$$d/ds(V_s[i]) = 2d\ quadrature(V_s[all\ j] , s)$$

Typically, we have to treat between 10.000 and 10.000.000 components -> Strategy:

- Store the array V[i] once within each single MPI task on a single node
- Within a single MPI task use OpenMP to parallelise the outer quadrature
- Within the inner quadrature we use symmetries of the model to increase data locality -> reduce computational effort and facilitate automatic vectorisation

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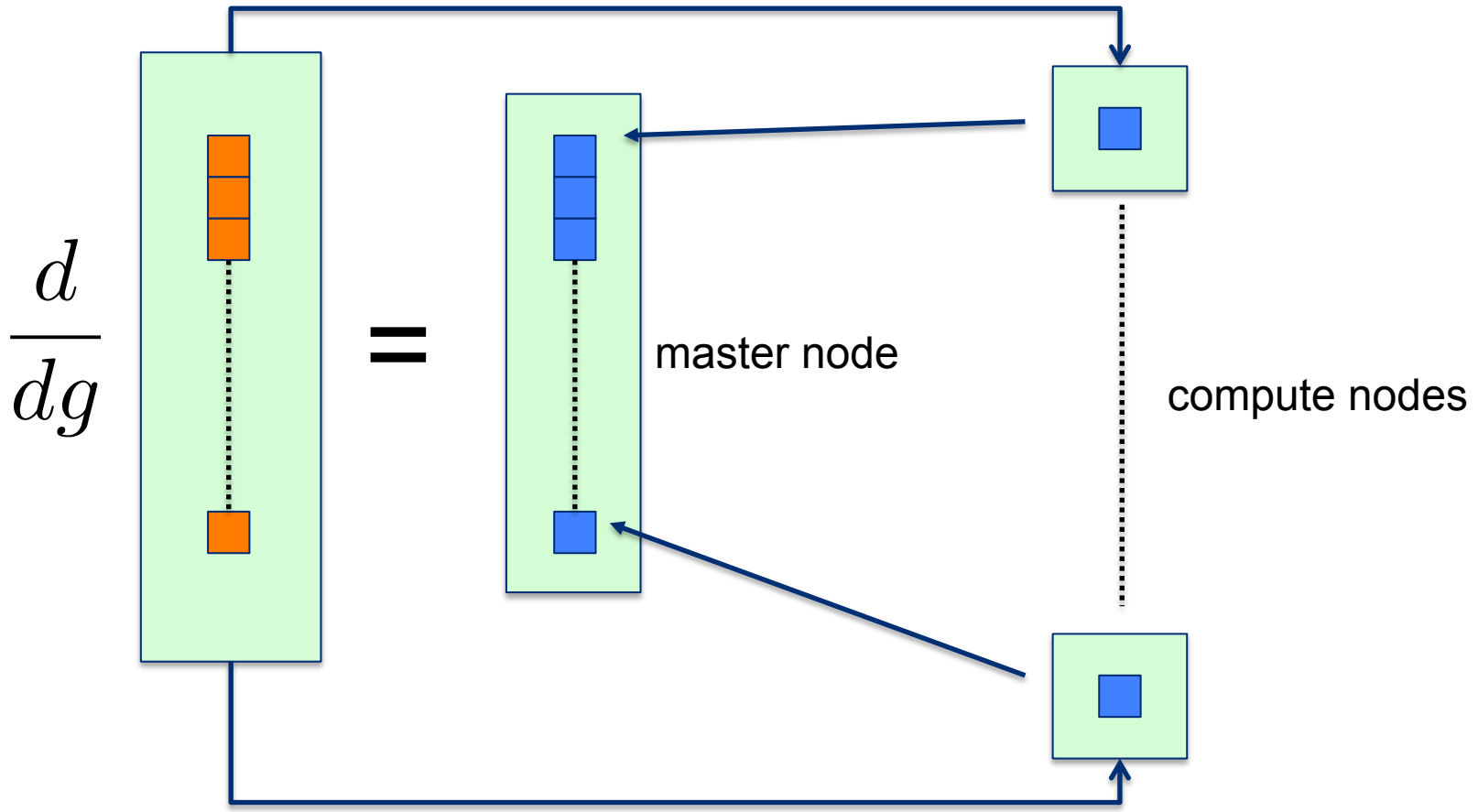
Technical Task: Solve large ODE



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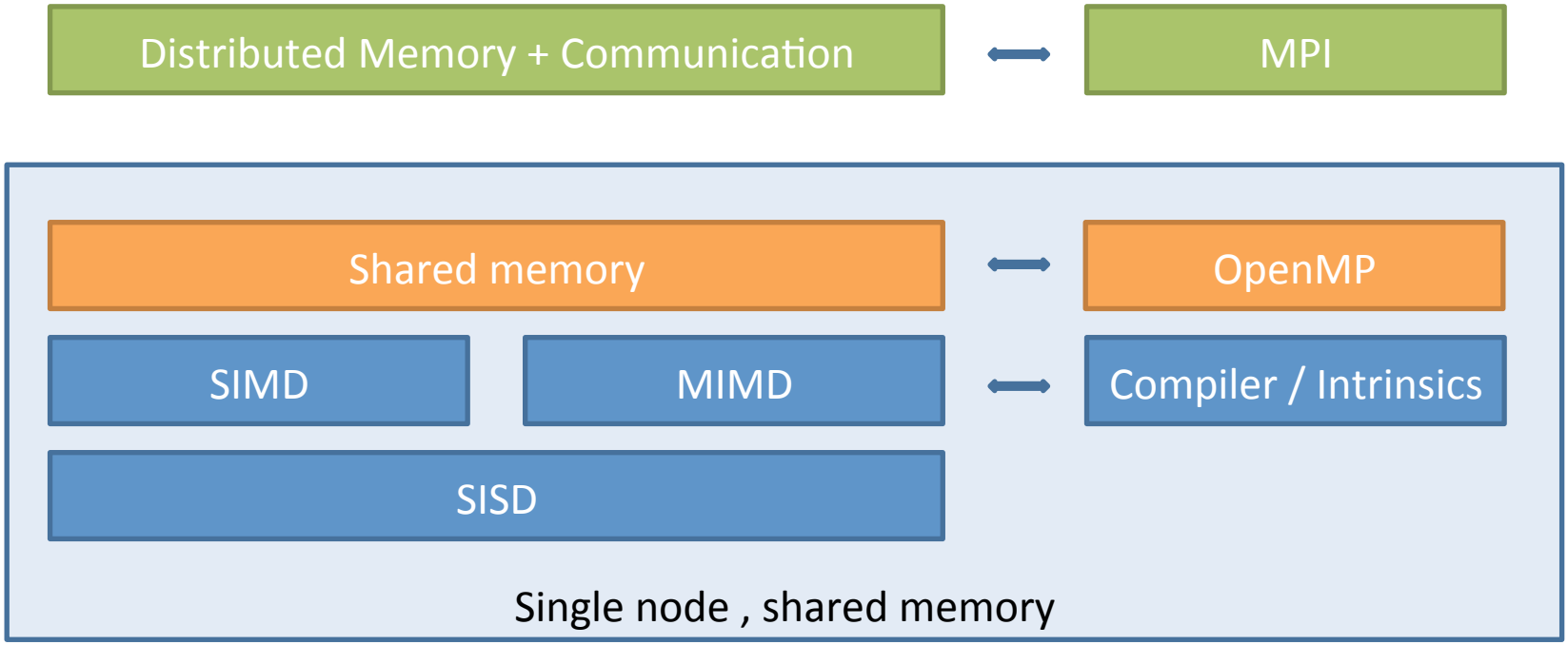
Hierarchical Hardware Environment



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Starting Point 2013

Code base

- legacy code which made use of MPI and scaled to about 64 single-core (!) nodes
- no Open-MP
- no vectorisation

Tools at hand

- Scalasca/Score-P (developed in-house)
- Vampir
- Intel VTune and Inspector

Ultimate goal

- good scaling on JUQUEEN up to the full machine (seemingly very unlikely)

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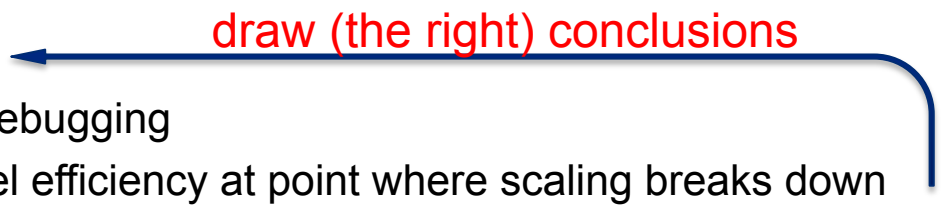
Work Plan

- adapt scheduling at highest level (MPI , distributed layer)
- implement shared memory parallelism at intermediate level (OpenMP)
- rewrite code at lowest level to allow for automatic SIMD-vectorisation

- cycle:
  - code change
  - benchmarking / debugging
  - analysis of parallel efficiency at point where scaling breaks down



- Central question: “How do we know why scaling brakes down at a certain point?”

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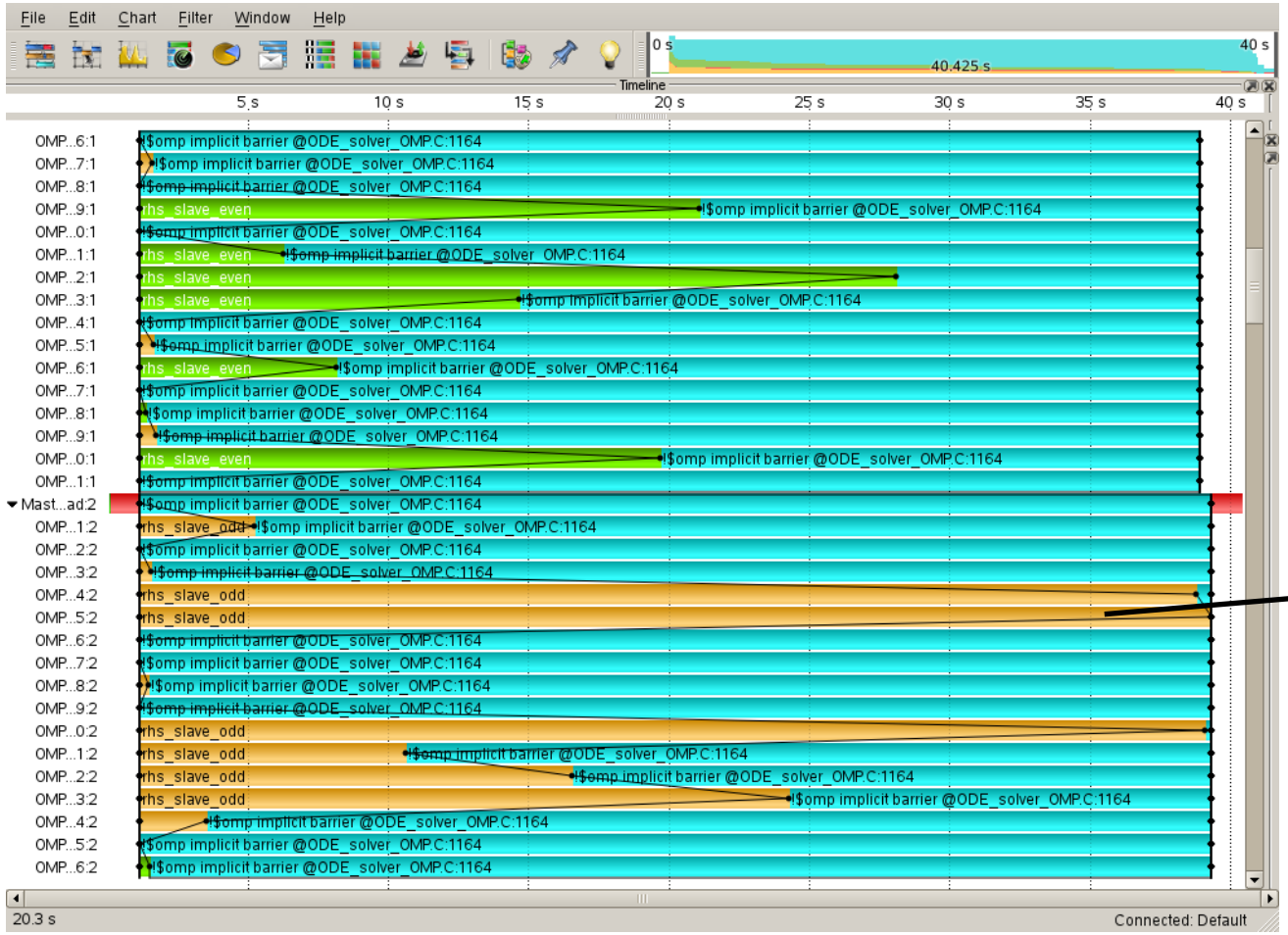
Visual Analysis 1: Poor efficiency



poor load-balancing

Screenshot taken from Vampir

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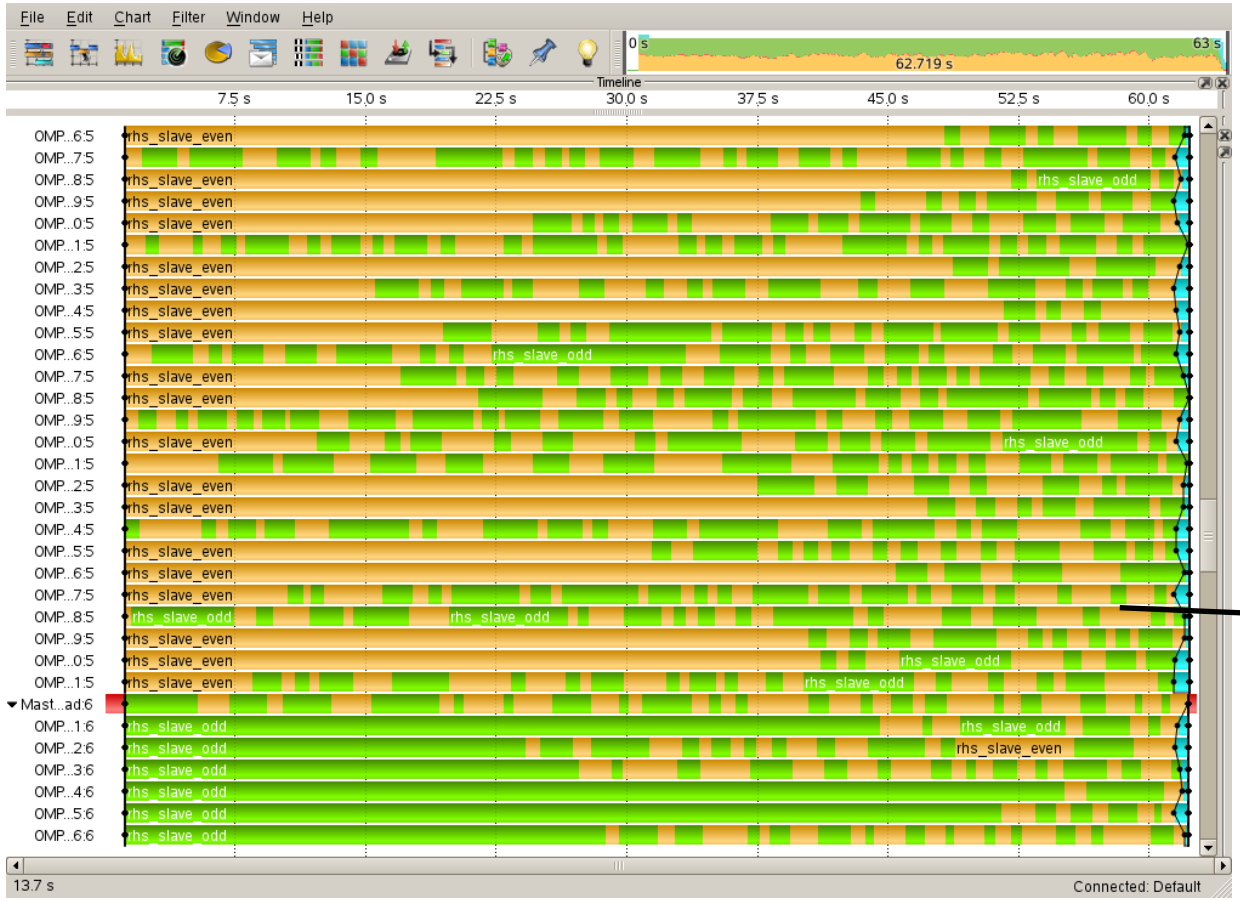
Visual Analysis 2: Good efficiency



good
load-balancing
(two time scales)

Screenshot taken from Vampir

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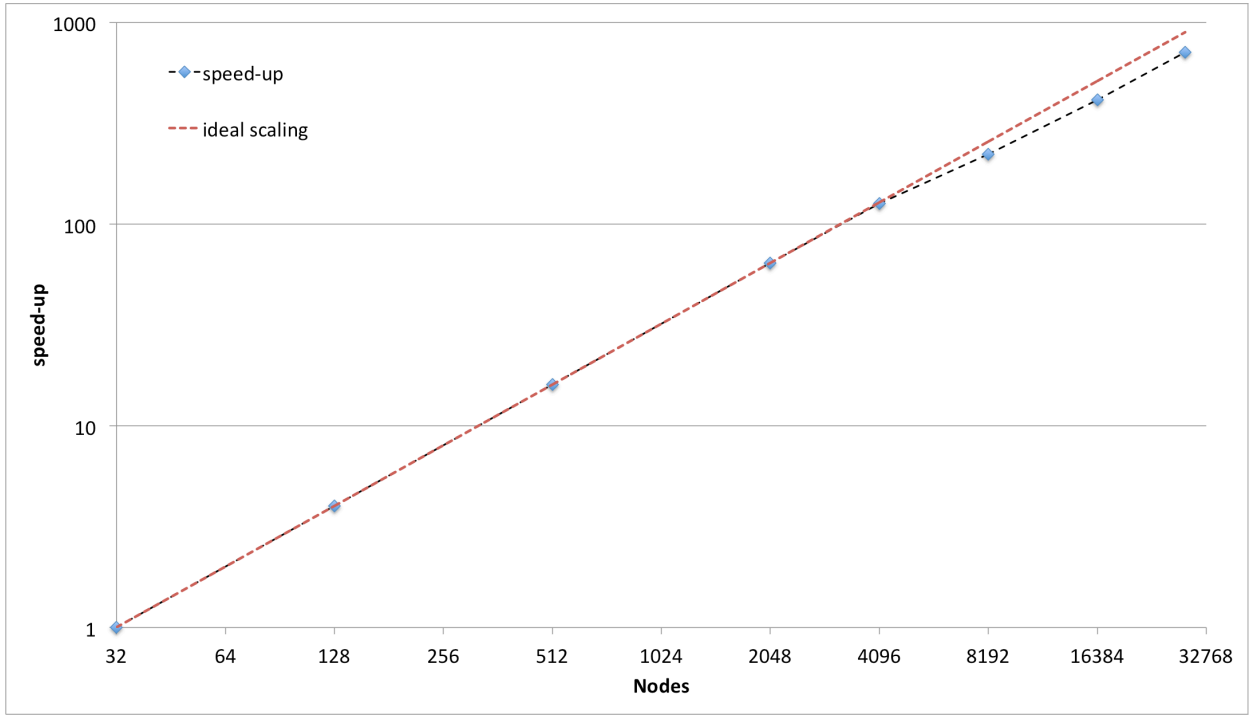
Status by the end of the project on JUQUEEN



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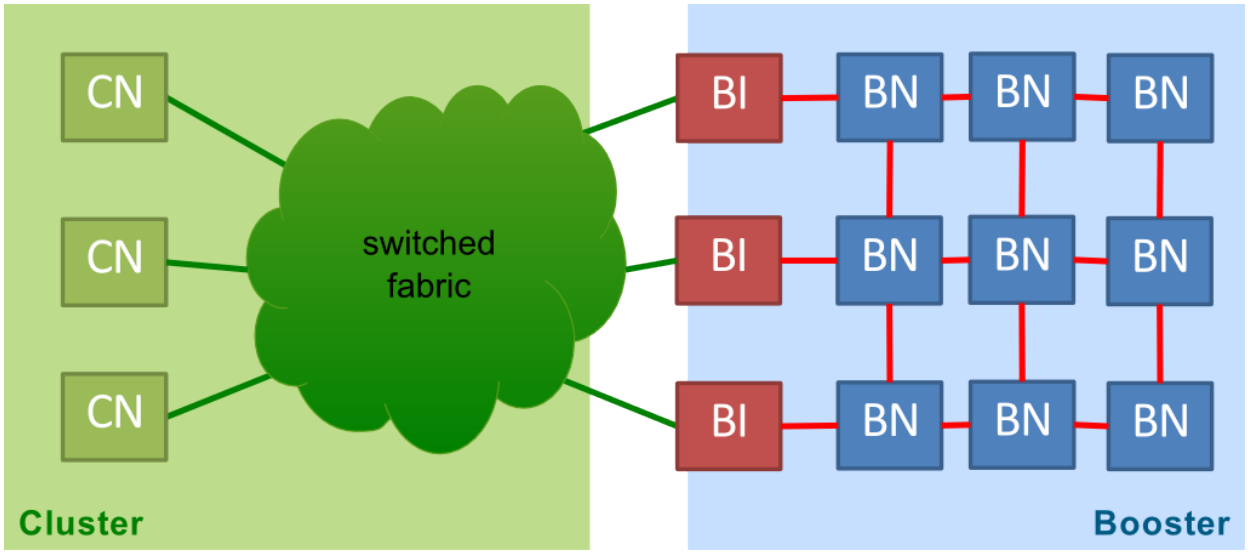
hp-fRG and Modular Computing on DEEP

The master-worker concept we use is the simplest setup which can profit from modular computing environments, where different parts of the code or even different codes within a larger computational framework run on different but highly connected infrastructures.



Quelle: DEEP Project

master task(s)

worker tasks

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Summary

The cross-sectional team “Application Optimisation” offers help and assistance in the process of tuning scientific codes on highly parallel HPC systems here at JSC.

We do this in close collaboration with the cross-sectional team “Performance Analysis” who develops and deploys HPC tools that are essential to our work.

We used an internally available code-base to conduct this exercise and to provide a demonstration of the potential of such a tuning process.

The effort-to-benefit ratio was very favourable.

The new code allows to extend scientific use-cases.

The new code is prepared to make use of modular computing environments.

Others have joined in: arXiv:1604.06296 , arXiv:1610.09991

More details in
Hierarchical parallelisation of functional renormalisation group calculations — hp-fRG
Computer Physics Communications Volume 207, October 2016, Pages 160–169
http://dx.doi.org/10.1016/j.cpc.2016.05.024

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Closing Message

Interested?

contact us at sc@fz-juelich.de

Thank you for your attention

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